Empirical Atomic Level Simulations for QC Applications

Paul von Allmen

Jet Propulsion Laboratory
California Institute of Technology

Contributors:
Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck
Jet Propulsion Laboratory
Tim Boykin
Univ. of Alabama, Huntsville

Collaborators:
Bob Joynt, Mark Friesen
Univ. of Wisconsin, Madison

Charter

1) Build simulation tools that help in designing QC in solid state implementation

2) Assist experimental efforts in characterizing and designing QC structures

Tools

1) Empirical tight binding electronic structure calculation software that can simulate systems with millions of atoms, strain, Coulomb interaction, magnetic field, optical properties
   NEMO-3D

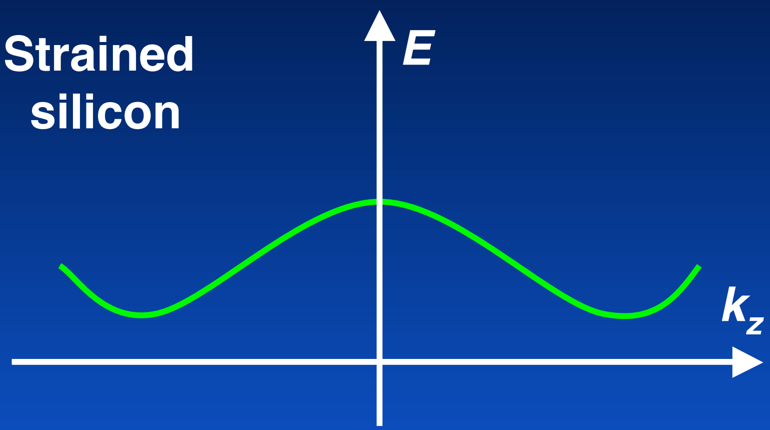
2) Quantum transport simulator using non-equilibrium Green function formalism; phonon scattering, interface roughness, alloy disorder, atomic level resolution, spin effects (under construction) and magnetic field (under construction)
   NEMO-1D and extension

Outline

1. Atomic level simulation of SiGe
2. Quantum confinement induced intervalley coupling in Si
3. Electrostatically defined quantum dot - 3D atomic level
4. Spin transport with non-equilibrium Green function
5. Atomic level simulation of quantum dot in magnetic field

Quantum confinement induced intervalley coupling in Si

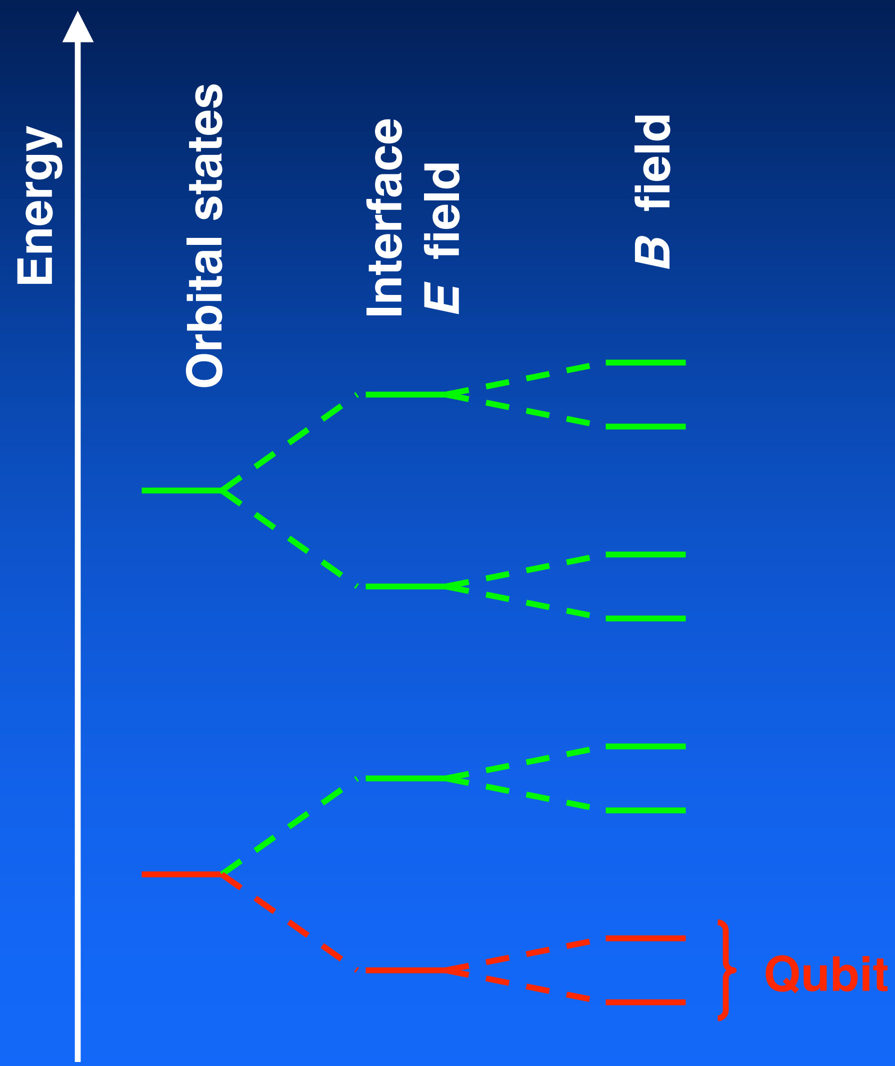
Strained silicon



Valley degeneracy in X direction is broken by interface and electric field

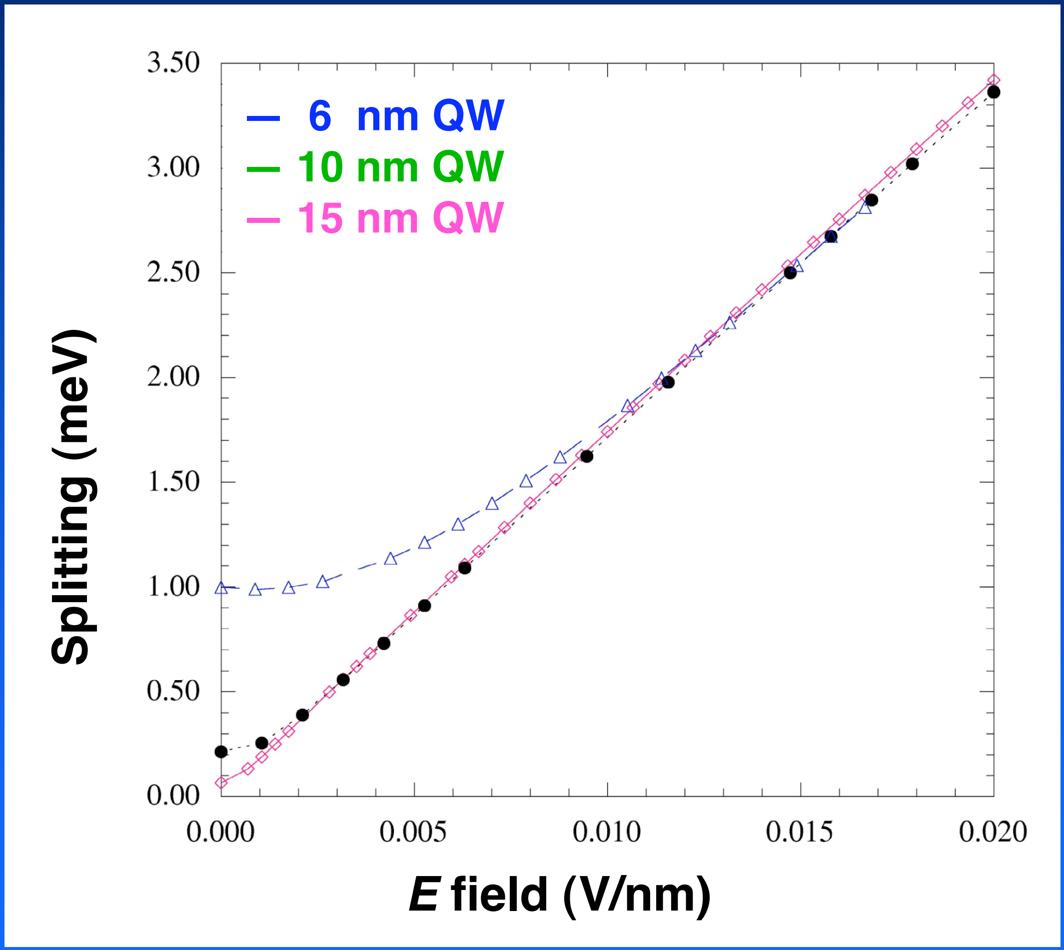
Are the qubit states separated enough from higher energy states?

Collaboration with University of Wisconsin



Quantum confinement induced intervalley coupling in Si

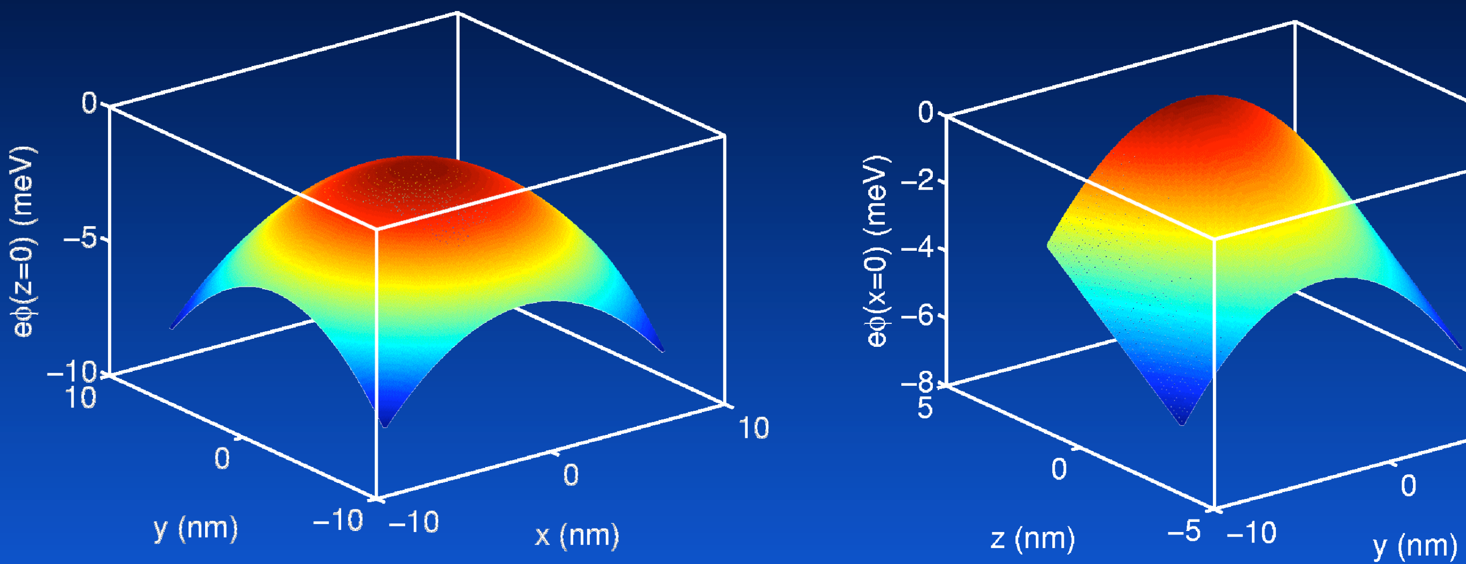
- 1D Tight Binding (NEMO 1-D)
- Si quantum well
- Strained on $Si_{0.8}Ge_{0.2}$
- Hard walls



Splitting is large enough (0.5-1.5 meV) for quantum computing

Collaboration with University of Wisconsin

Electrostatic confinement in Si QW

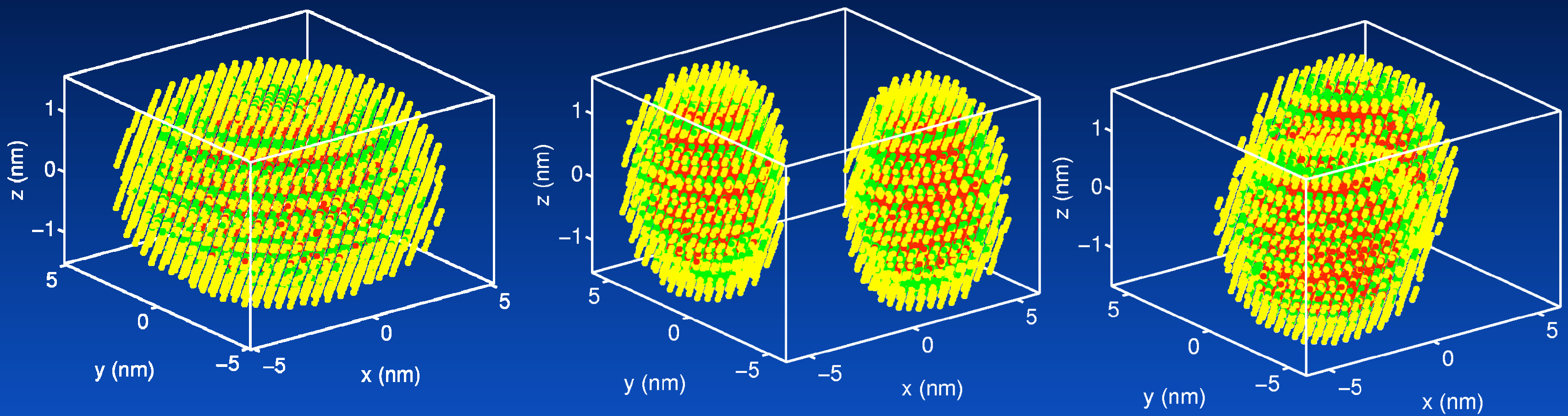


Geometry

- 5nm Si quantum well lattice-matched to $Si_{0.8}Ge_{0.2}$ (0.8% tensile strain)
- Non-zero field along z and lateral electrostatic confinement.
- Rescaled problem size ($5x10^4$ atoms) from WI group

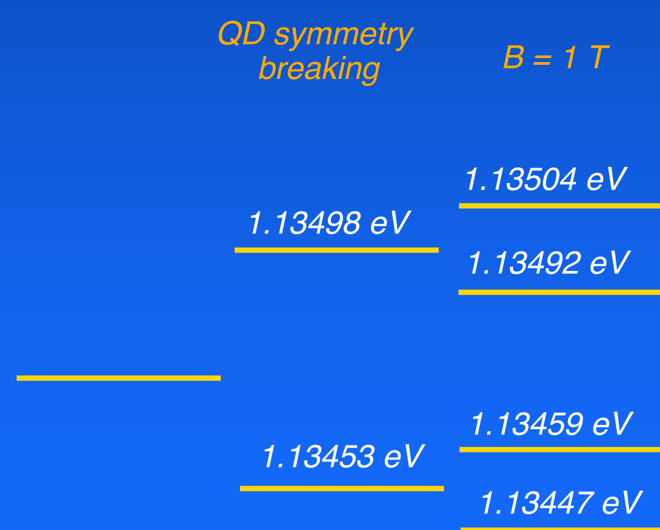
Collaboration with University of Wisconsin

Electronic structure of low-lying states



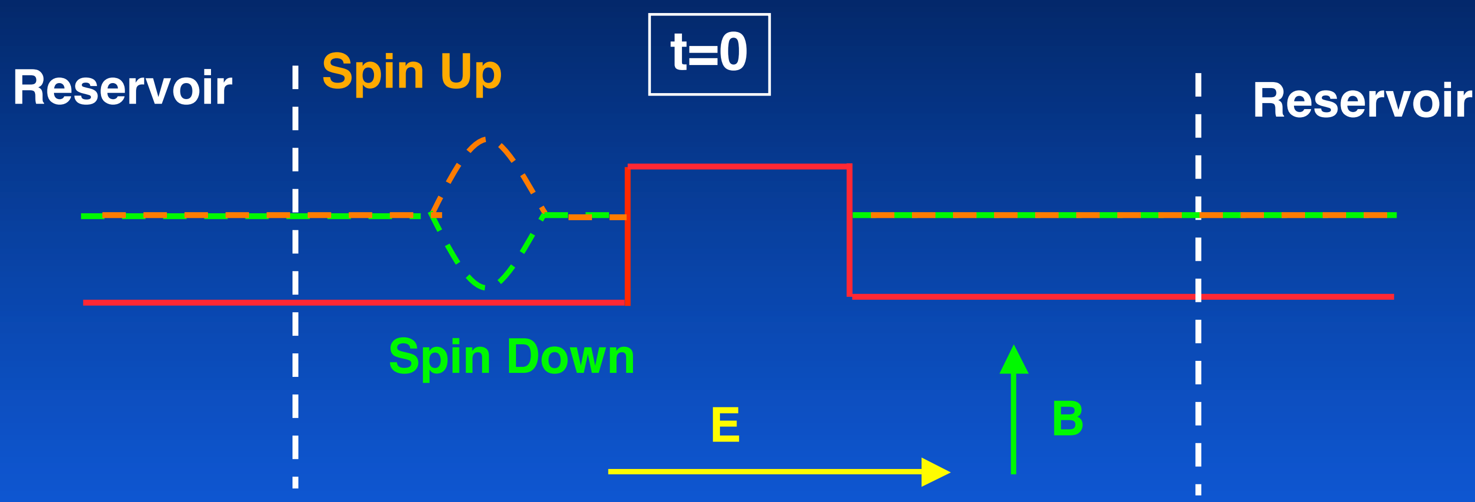
Splitting of electronic levels

- Valley splitting due to loss of translational symmetry in QD (~0.45 meV)
- Zeeman splitting is smaller (~0.12 meV).



Collaboration with University of Wisconsin

Spin Transport with Non-Equilibrium Green Functions



Time evolution

1. Spin transport
2. Spin precession
3. Spin relaxation and decoherence

Applications

1. Magneto-optic (TRKR) experiments
2. Transport between qubits
3. Preparation of initial state for QC

Spin Transport with Non-Equilibrium Green Functions

Equations of motion

$$\left(i\partial_t - H^{(0)}\right)G^<(xt,x't') = \int dx''dt''\,\Sigma^<(xt,x''t'')G^a(x''t'',x't') + \int dx''dt''\,\Sigma^r(xt,x''t'')G^<(x''t'',x't')$$

$$\left(i\partial_t - H^{(0)}\right)G^r(xt,x't') = \delta(t-t')\delta(x-x') + \int dx''dt''\,\Sigma^r(xt,x''t'')G^r(x''t'',x't')$$

$$H^{(0)} = \frac{p^2}{2m} + V(x) - \mu B\cdot S$$

Open boundaries (finite difference or tight binding)

$$\left(i\partial_t - H^{(0)}_{nm}\right)G^<_{mn'} = \delta_{n1}\Sigma^{Br}_{11}G^<_{1n'} + \delta_{n1}\Sigma^{B<}_{11}G^a_{1n'} + \delta_{nN}\Sigma^{Br}_{NN}G^<_{Nn'} + \delta_{nN}\Sigma^{B<}_{NN}G^a_{Nn'}$$

$$\left(i\partial_t - H^{(0)}_{nm}\right)G^r_{mn'} = \delta_{nn'} + \delta_{n1}\Sigma^{Br}_{11}G^r_{1n'} + \delta_{nN}\Sigma^{Br}_{NN}G^r_{Nn'}$$

$$\Sigma_{11} = H^{(0)}_{10}G^0_{00}H^{(0)}_{01}$$

$$\Sigma_{NN} = H^{(0)}_{NN+1}G^0_{N+1N+1}H^{(0)}_{N+1N}$$

Surface Green Functions

1. Stationary in time (NEMO-1D)
   - Fourier transform of Green function
   - Algebraic Dyson equation
   - Recursive method to calculate the surface Green function

2. Time dependent case

$$G_{00}^{<0}(t,t') = g_{00}^{<0}(t-t')M^{<}(t,t')$$

$g_{00}^{<0}(t-t')$ is the surface Green function for a spinless system

$$M^{<}(t,t') = \begin{pmatrix} \cos\frac{\omega_L t}{2}\cos\frac{\omega_L t'}{2} & -i\cos\frac{\omega_L t}{2}\sin\frac{\omega_L t'}{2} \\ -i\sin\frac{\omega_L t}{2}\cos\frac{\omega_L t'}{2} & \sin\frac{\omega_L t}{2}\sin\frac{\omega_L t'}{2} \end{pmatrix}$$

$$\omega_L = \gamma B$$

Polarized spin up

Tight-binding model for magneto-optical response

- **Gauge-invariant modification of tight-binding Hamiltonian**
  [M. Graf and P. Vogl , Phys. Rev. B **51**, 4940 (1995)]

$$\square_i = \square_i^0 + \square_B B \cdot \square$$

On-site interaction

$$t_{ij} = t_{ij}^0 \exp(\square \frac{ie}{hc} \square_{R_j}^{R_i} A \cdot dr)$$

Nearest-neighbor interaction

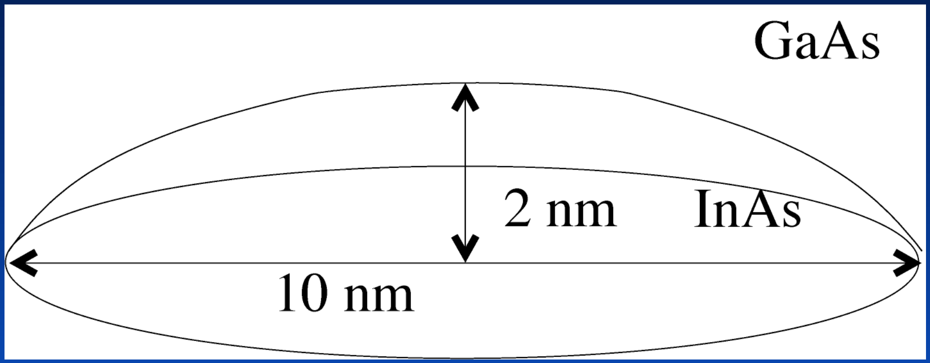
- **Absorption rate between conduction and valence levels**
  [S. Lee et al., Phys. Rev. B **66**, 235307 (2002)]

$$\square(E) = \frac{2\square}{\hbar} \left| \langle c \mid \hat{r} \mid v \rangle \right|^2 \square(E_c \square E_v \square E)$$

$$\langle c | \hat{r} | v \rangle = \square_{ij} c_j^* v_i \left[\hat{r}_i \square_{ij} + \langle j | \square \hat{r}_i | i \rangle \right]$$

InAs self-assembled lens-shaped dot

- **Modeled system geometry**



- **Strain profile model: atomic elasticity model**

  [P. N. Keating, Phys. Rev. B **145**, 637 (1966)]

  Strain energy as a function of bond length and bond angle.

- **Tight-binding Hamiltonian**

  Basis orbitals: $sp^3d^5\,s^*$

  Parameters generated by a genetic algorithm.

  Size : 921600 = 46080 atoms X 10 basis orbitals X 2 spins

- **Eigenvalue solver: Arnoldi method with PARPACK package**

  Computation on a Beowulf cluster with 30 nodes.

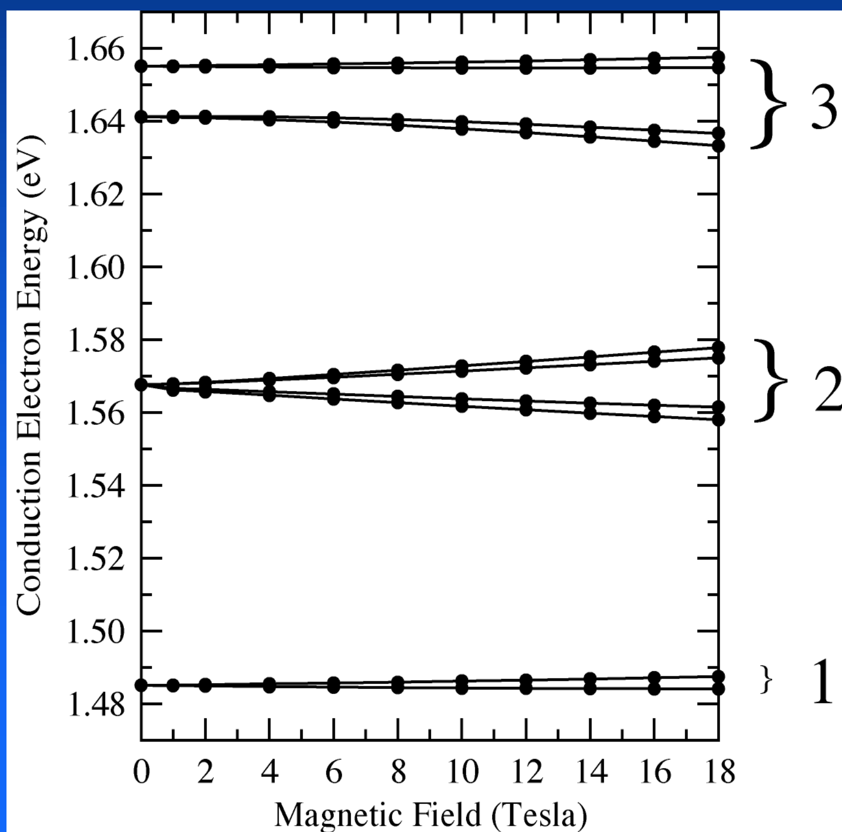
Magnetic-Field Effect on Electronic Structure of InAs Dot

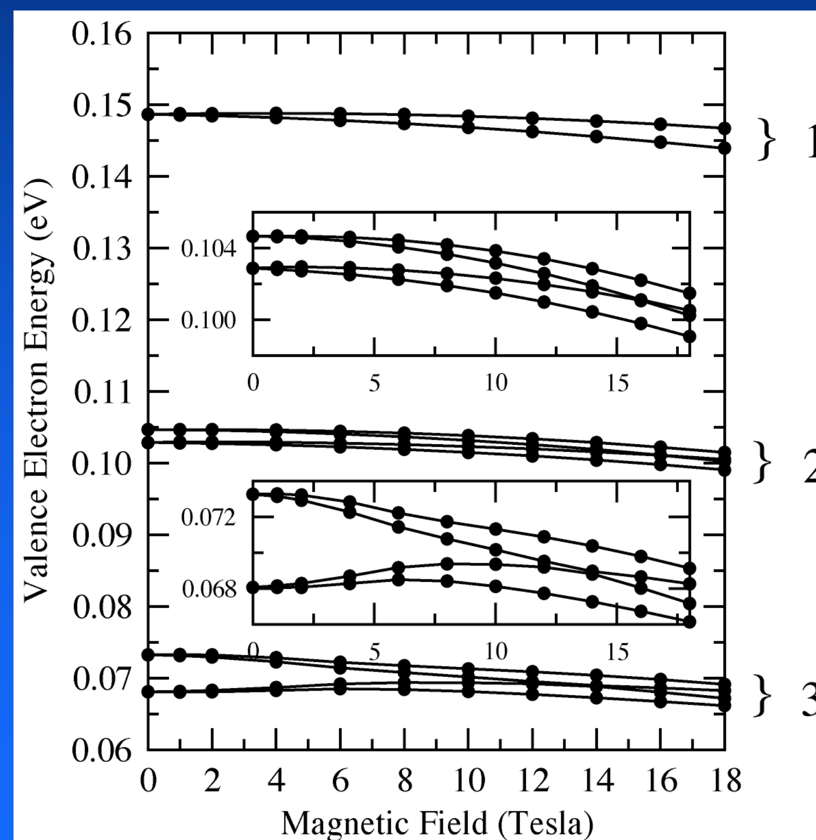
Conduction Electron Levels

- Zeeman Interaction splits the levels into spin-up and -down levels.
- Effective g-factor ($g = (E_{\uparrow} - E_{\downarrow})/\mu_B B$) ranges from 2 to 3.5.

Valence Electron Levels

- Zeeman interaction splits the levels into Jz = 3/2 and Jz = - 3/2 levels.
- Zeeman interaction couples closely-spaced levels.





Magneto-Optical Response of InAs Quantum Dot

- Selective dipole coupling between electron and hole levels.
- The selectivity remains intact even at a high magnetic field.

$$\Delta L = 0 \ \& \ \Delta j = 1$$